

# 1-Nitrobutane

627-05-4 | DTXSID8020967

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** -11.9 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 6.95e-01

**Confidence level:** 7.70e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

1-Nitrobutane

**Measured:** -11.8

**Predicted:** -11.9

[Image not found](#)

N-Butylnitrite

**Measured:** -11.6

**Predicted:** -11.7

[Image not found](#)

1-Nitropropane

**Measured:** -12.4

**Predicted:** -12.2

[Image not found](#)

2-Nitropropane

**Measured:** -12.6

**Predicted:** -12.4

[Image not found](#)

Butyl nitrate

**Measured:** -11.8

**Predicted:** -11.8